Technological Aspects of Development of the Web-trainer on Crystallography

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Abstract

The given work is devoted to creation "Crystal" web informational educational handbook on crystallography and mineralogy. The presented set of data for each mineral excels the similar ones. Algorithms to crystal visualization by its mineralogy representation are developed, the computational efficiency optimized. The "Crystal" web-trainer is used in educational process of Novosibirsk State University.

1. Introduction

Informational and educational Web-based training system "Crystal" was created to solve the problem of sharing the various important information about crystals and minerals and to help one to explore and use the geological data. There are some recent researches and developments on this subject, which also have free access through the Internet (see [1, 2,]), e.g., some mineralogical databases intended for scientific and educational purposes, but the information which is provided by those databases is definitely specific.

Web-based training system "Crystal" is the web site with applications, systematized facts, and references from the fields of mineralogy, crystallography and crystal optics, supplemented with series of examples and realistic images. The information had been gathered from different sources or had been achieved by the authors. Some sources become rare books today. Thus web-trainer has solved the problem of increasing a lack of *bibliographic* sources.

This work is the third stage of development of the trainer "Crystal". The first stage was discussed in [9] as the case study and reflects the geologists' view of the WEB-trainer. The only of 32 symmetry groups of crystals was considered there. The next stage involved all groups of symmetry and was published in [8].

Web-trainer provides the access to the following resources:

- Data base including the full information from crystallography, mineralogy, crystal optics, geochemistry about more then a hundred minerals;

- Theoretical information from crystallography and mineralogy;

- The editor allowing to create and modify the crystal models.

While developing the "Crystal" web-trainer the authors encountered the following requirement: all incoming information is in the format that is geological standard, and is familiar to any geo-scientist. This requirement made the additional difficulty to use incoming mineralogical information as source data for graphical output.

"Crystal" is used in educational process of Geological Dept. of Novosibirsk State University since year 2000. It is necessary to note that trainer has changed teaching methods radically. In past times 3D models of wood and cardboard were made by students or teachers for better understanding crystal geometry. It took significant time to calculate and glue or fashion this kind of models from paper of wood.

Nowadays students of Novosibirsk State University are provided with allotted time in the terminal classrooms for self-education using "Crystal" training systems. They can study geometry and characteristics of the 3d crystal models or do geological exercises mouse and keyboard in order to represent 3D geometric data. The "Crystal" web trainer is available at Novosibirsk State University Web-site http://ggd.nsu.ru/Crystal/.

2. "Crystal" web-trainer structure

From the technical standpoint web trainer is a complex system consisting of several program components. These components are mineralogical database, web interface providing access to the database, and crystal 3d models constructor. Principle of the components interaction is shown in Fig. 1: a *user* is provided with access to the remote *database* through the *web-interface*.
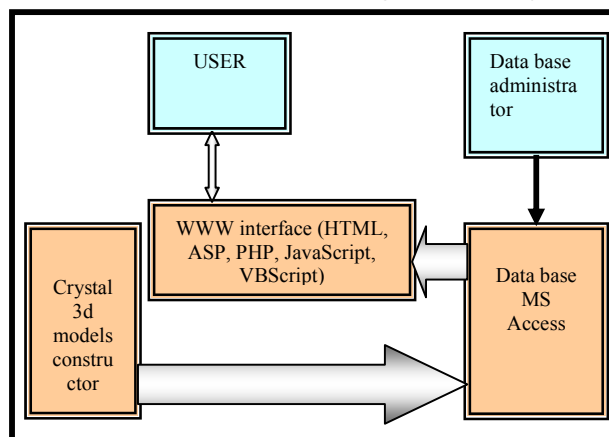

Figure 1: Web-trainer structure

Crystal 3d models constructor helps to work with geometric information on minerals on the base of visual feedback, particularly, it is used for database replenishment with new data related to geometric construction of crystals.

Note that database is a main component of our web trainer, due to the fact that all information on minerals, their characteristics resides at this database and necessary data is sent to client part as HTML code when the Web-interface queries the data. Thus it is not necessary to create the separate HTML document for each mineral. That makes the process of adding new minerals to the Web-trainer significantly easier.

2.1. Database

New universal and compact form of the full description of the mineral properties was developed for "Crystal" web-training system. This form allowed storing these descriptions in the database.

RDBMS Microsoft ® Access was used for managing and maintaining the database.

Our database is unique among different mineralogical databases. The point is that usually mineralogical databases store information that is specific for certain field of research. The database used in the Web-training system "Crystal" contains the information on more than a hundred minerals used in different sciences dealing with minerals: physics, chemistry, geometry, mineralogy (elementary cell parameters, type of crystal symmetry, twinned crystals, simple forms, Miller indexes, etc). Database is very important and valuable itself because it surpasses other existing geological databases available at the world market.

The database contains MS Access forms that facilitate the entering and updating the data on minerals. The way data is published in the Internet is discussed in the "Web-Interface" section of this paper.

2.2. Crystal 3D models constructor

Crystal 3D models constructor is a standalone Win32 application that uses Microsoft DirectX technologies for realistic visualization of crystal models being edited. This technology is discussed in detail in [2].

The input and output data for 3D models constructor is traditional **mineralogical description** of the crystal geometry (convex polyhedron). Mineralogists usually use the following way for defining the crystal geometry: the oblique-angled coordinate system is specified at first, and then the normal vectors of crystal faces are defined in this coordinate system along with the distances from the coordinate system origin. The coordinate system basis is defined according to the main directions of the lattice of the crystal [1].

While development of the Crystal 3D models constructor application the algorithm was invented that converts the mineralogical description of the crystal geometry into the conventional representation of the convex polyhedron as the set of vertexes, edges and faces. This algorithm and other features of this application development can be found in [4].

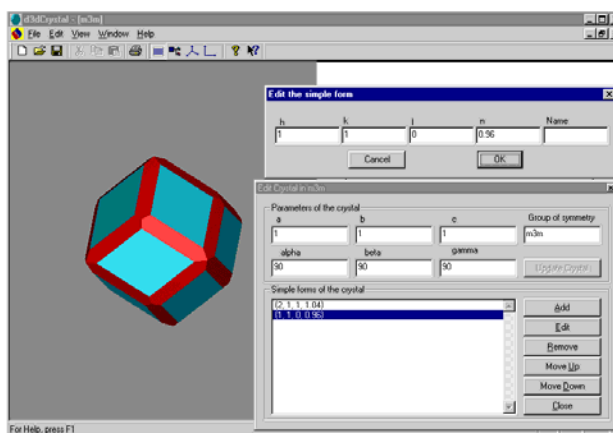Fig. 2 represents the user interface of the Crystal 3D models constructor application.

Figure 2: Crystal 3D models constructor GUI

A lot of crystals have complicated geometry, that is why even minor inconsistency or incorrectness of the input mineralogical description of the crystal can affect the geometry of the crystal drastically. The Crystal 3D models constructor allows changing of the crystal mineralogical description interactively. A user can see how the changes he/she makes to the mineralogical description influence the geometry of the crystal.

2.3. Web Interface

Web interface of the training system is based on ASP (Active Server Page) technology and includes server and client sides (see [5]). Server side retrieves the data from the MS Access database using ADO (ActiveX Data Objects). The database resides at the same server machine. The server side also creates HTML-pages based on the information from the database. These HTML pages are sent to the client side by request.

The HTML pages represent text and graphical information about certain crystals and also contain Java-applets. Text provides the information about chemical, physical and geometrical properties of the minerals. Graphical part includes the photographs, drawings and 3D crystal models. For representing the 3D crystal models Java applets are used.

Web interface provides also database search capabilities. Search can be performed for the mineral name or its crystallographic properties such as elementary cell parameters or the type of symmetry.

Most of the pages are expanded with theoretical information from crystallography and mineralogy.

2.3.1. Applets

Good spatial reasoning is needed for understanding of a crystal shape. Classic educational process in mineralogy provides a study of a crystal shape by a model made of wood, cardboard, or wire. Authors use Java programming language in order to provide better visualization of crystallography information: crystal models are built as dynamic graphical objects, which can be handled with mouse.

A crystal can be defined in two ways: either as a set of the faces in oblique frame or as stereographical projection (special representation of a solid object on the plane). A purpose of the work was to create algorithms:

- Conversion from mineralogical notation to conventional one, e.g., vertices and edges,
- Drawing of stereographical projection of a cristal.

At the first step of development the "Crystal" web-trainer contained minerals of one type of symmetry only. Nature minerals can be of one of 32 symmetry groups. The rules of correspondence between a symmetry group and a crystal faces were defined in this work. Applets based on these rules were created, which model all real minerals of all 32 symmetry groups.

This work includes developments of:

- The Interactive Visualizer. It is used for visualization of 3D crystal models and its stereographical projection using mineralogical data. In Fig. 3 one can see its user interface.

- Interactive Elementary Cell Builder. It draws elementary cells of crystal tessellation based on mineralogical data. (Fig. 5).
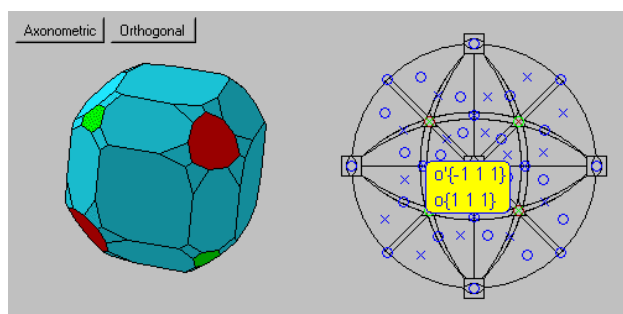

Fig 3: *3D model of boracite crystal*

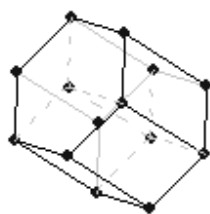**Fig 4.** *Photo of boracite crystal*

Fig 5. *Elementary cell model*

3. Computation speed estimates

A basic algorithm to build 3d model of crystal from mineralogical data is a full look-through algorithm. It means that if a crystal has N faces than an algorithm fulfills:

- N^2 comparisons of faces to avoid doubling – second order algorithm.

- N^4 operations to find crystal vertices – fourth order.

In fact the implemented algorithm requires maximum 12 seconds to load applet, to perform all calculations, and to show a picture on the screen. Note that the given implementation fulfills all manipulations without any visible delays.

4. Conclusion

Developed handbook has convenient GUI, that allows user to deal with the next resources:

- Database that including whole crystallographical, mineralogical information as well as some crystal optics and geochemistry characteristics of more then 100 minerals.

- Theoretical information and lectures on crystallography and mineralogy.

- Crystal Builder and Editor.

Models built can be viewed from any point and can be handled using a mouse. So, educational efficiency of learning the handbook is at least the same, as the efficiency of work with classic crystal models made of wood and metal.

"Crystal" web-trainer is developed with the help of Novosibirsk Regional Center of Geoinformational Technologies (http://www.giscenter.ru), it has real users and application area (it is being used at Novosibirsk State University (http://www.nsu.ru)).

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Аннотация

Данная работа посвящена созданию web-справочного учебного пособия по кристаллографии и минералогии «Кристалл». Представляемый набор данных по каждому минералу превосходит аналоги. Разработаны алгоритмы визуализации кристаллов по минералогическому представлению, выполнена оптимизация по скорости вычислений. Пособие применяется в учебном процессе в Новосибирском государственном университете..